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Approximation for the enhancement factor applicable to reversible reactions of finite rate in chemically loaded solutions

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Abstract—A new explicit relation is proposed for the prediction of the enhancement factor for reversible reactions of finite rate in chemically loaded solutions which also allows for unequal diffusivities. The relation for the enhancement factor is not based on an approximation of the absorption process, but is derived from a similarity which can be observed between the results of the approximation for an irreversible (1,1) order reaction given by, for example, DeCoursey (surface renewal model), and the exact numerical results. The present relation combines the solution of DeCoursey (1974 *Chem. Engng Sci.* **29**, 1867–1872) for irreversible finite rate reactions, and the solution of Secor and Beutler (film model, 1967 *A.I.Ch.E. J.* **13**, 365–373) for instantaneous reversible reactions. The diffusivity ratios in the solution of Secor and Beutler (1967) were replaced by the roots of these ratios in order to adapt the enhancement factors to the penetration theory. In general, this adaptation of the solution of Secor and Beutler gave reasonably good results, however, for some situations with unequal diffusivities deviations up to 20% were found. The results of the present approximation were for various reactions compared to the numerical enhancement factors obtained for the model based on the Higbie penetration theory. Generally, the agreement was reasonably good. Only 26 of 2187 preselected simulations (1.18%) had a deviation which was larger than 20%, while the average deviation of all simulations was 3.3%. The deviations increased for solutions with a substantial chemical loading in combination with unequal diffusivities of the components. For reactions with a kinetic order unequal to unity, the Ha number had to be multiplied by a factor, $\sqrt{f}$, so that $E_a = \sqrt{f}\,Ha_A$ in the regime $2 < Ha_A \ll E_{a,\infty}$. This factor agreed well with the factor given by Hikita and Asai (1964, *Int. Chem. Engng* **4**, 332–340) in their dimensionless number. © 1997 Elsevier Science Ltd.

Keywords: Gas absorption; modelling; enhancement factor

1. INTRODUCTION

In gas–liquid absorption processes the enhancement factor concept is introduced to describe the influence of a reaction on the mass transfer rate. The enhancement factor is defined as the ratio of the rate of absorption of a gas in a reactive liquid to the rate of the physical process at identical concentration differences of the absorbing gas. Since the occurrence of a chemical reaction can have a substantial effect on the absorption rate, a good description of this phenomenon is required for design purposes. Therefore, much attention has been paid to the description of gas absorption in reactive liquids.

For these phenomenon a large number of theoretical models are proposed (see, e.g. Versteeg *et al.*, 1989). Three frequently encountered models are the film theory, Higbie penetration theory and the Danckwerts surface renewal model. The effect of the chemical reaction is usually described by the implementation of the chemical reaction in these mass transfer models (see e.g. Danckwerts, 1970). As mentioned before, the results of the incorporation of the influence of the reaction on the mass transfer rate are usually presented in terms of the enhancement factor. Glasscock and Rochelle (1989) showed that, for the models mentioned, considerable differences for the numerically calculated enhancement factors could occur at identical process conditions. The differences between the penetration and surface renewal model were generally small, while the film model showed larger deviations. Generally, the film model is regarded as the most simplified and, therefore, physically most unrealistic model. Therefore, the enhancement factor obtained with either the model based on

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the penetration theory or the model based on the surface renewal theory will be preferred.

Only for some asymptotic absorption processes accompanied with chemical reaction the different absorption models can be solved analytically, while for all other situations numerical solutions are necessary (see, e.g. Swaaij van and Versteeg, 1992). As the numerical solution of the mass transfer model is laborious, various approximations were developed to estimate the enhancement factor, which are applicable over a wide range of process conditions, reversible reactions and chemical solute loadings. Well-known examples, among others, are the pioneering work of van Krevelen and Hoftijzer (film model), the solution of Onda *et al.* (1970, film model) and DeCoursey (1974, 1982, surface renewal theory). DeCoursey and Thring (1989) eventually produced an implicit approximation which was based on the surface renewal model which took allowance for all possible conditions of reaction (1), with first-order kinetics in the gas A and reactant B.

$$\gamma_a A + \gamma_b B \Leftrightarrow \gamma_c C + \gamma_d D \tag{1}$$

With this approximation enhancement factors can be calculated relatively easily. Recently, Winkelman *et al.* (1992) compared the solution of DeCoursey and Thring to the results obtained with a numerical model based on the Higbie penetration theory. For chemically unloaded solutions, the maximum deviation was 11% (average deviation 2%), while for chemically loaded solutions this value increased up to 14% (average deviation 3.1%). Although the model of DeCoursey and Thring allows for all possible stoichiometric combinations for reaction (1), the reaction must be first order in the gas A and reactant B, which can be considered as a severe restriction.

In the present contribution a simple explicit relation for the enhancement factor is presented which is not based on the approximation of the absorption process, but it is derived from a similarity which can be observed between the results of the approximation of, e.g. van Krevelen and Hoftijzer or DeCoursey (1974), and the exact numerical results. The enhancement factors obtained with this relation for various kinetic expressions will be compared to the exact results calculated with a numerical model which is based on the Higbie penetration theory.

2. THEORY

2.1. *Basic relations of film model*

Although the final approximation is valid for reversible reactions and the penetration model first the irreversible reaction

$$A + \gamma_b B \Rightarrow \gamma_c C + \gamma_d D \quad \text{with } R_a = -k_{n,m}[A]^n[B]^m \tag{2}$$

is considered to derive an expression for the dimensionless Hatta number. For a correct description of the fluxes according to the film model the following dimensionless equations have to be solved:

$$\frac{d^2\alpha}{d\zeta^2} = Ha_A^2 \alpha^n \beta^m, \qquad \zeta = 0, \quad \alpha = 1 \quad \text{and}$$

$$\zeta = 1, \quad \alpha = 0 \tag{3}$$

$$\frac{d^2\beta}{d\zeta^2} = Ha_B^2 \alpha^n \beta^m, \qquad \zeta = 0, \quad \frac{d\beta}{d\zeta} = 0 \quad \text{and}$$

$$\zeta = 1, \quad \beta = 1 \tag{4}$$

with

$$\zeta = x/\delta \quad \alpha = [A]/[A]_i \quad \beta = [B]/[B]_L \tag{5}$$

in which the dimensionless number Ha_A is defined by

$$Ha_A^2 = \frac{k_{n,m}[A]_i^n [B]_L^m \delta}{\frac{D_a}{\delta}[A]_i} = \frac{k_{n,m}[A]_i^{n-1}[B]_L^m D_a}{k_L^2} \tag{6}$$

and the dimensionless number Ha_B is defined by

$$Ha_B^2 = \frac{\gamma_b k_{n,m}[A]_i^n [B]_L^m \delta}{\frac{D_a}{\delta}[B]_L} = \gamma_b Ha_A^2 \frac{D_a}{D_b}\frac{[A]_i}{[B]_L}. \tag{7}$$

Note that both the Ha_i^2 numbers in fact represent the maximum conversion of component i in the film divided by the maximum transport of component i through the film. In this way the Ha_A number coming from the dimensionless relation has a distinct physical meaning. If $m = 0$, i.e. a zeroth-order reaction in B, the Ha_A number is the only variable and the enhancement factor is a unique function of this Ha_A number.

For some asymptotic situations these coupled differential equations (3) and (4) can be solved analytically to derive the flux of A at the interface, however, in most situations, which include reversible reactions, numerical techniques or approximations are necessary in order to calculate the flux of A at the interface. These approximations often assume a profile of component B in order to simplify the differential equations and make them analytically solvable.

2.2. *Approximate solutions and derivation of the present relations*

Van Krevelen and Hoftijzer introduced a linearization technique for the concentration of B in the film model and obtained an implicit approximation for the enhancement factor for a second-order irreversible reaction (8):

$$A + \gamma_b B \Rightarrow C + D \quad \text{with } R_a = -k_{1,1}[A][B]. \tag{8}$$

With the general solution of van Krevelen and Hoftijzer the enhancement factor according to the film model can be calculated within 3% (Santiago de and Farina, 1970).

Brian *et al.* (1961) showed that by substituting the diffusivities by the square root of the diffusivities, the relation of Van Krevelen and Hoftijzer is also applicable to the the penetration theory for reaction (8) with deviations within 7% for a second-order irreversible reaction.

DeCoursey (1974) developed an explicit approximate relation for the enhancement factor for reaction (8) which was based on the surface renewal theory, while Yeremian *et al.* (1970) derived an approximate explicit solution according to the penetration theory. The solution of DeCoursey (1974) is given by

$$E_a = \frac{-Ha_A^2}{2(E_{a,\infty}-1)} + \sqrt{\left[\frac{Ha_A^4}{4(E_{a,\infty}-1)^2} + \frac{E_{a,\infty}Ha_A^2}{(E_{a,\infty}-1)} + 1\right]}. \quad (9)$$

The effect of the reversibility of the reaction has been shown by, among others, Versteeg *et al.* (1989) and is demonstrated in Fig. 1 for various values of the equilibrium constant. In this figure also the enhancement factor for the irreversible reaction (8) according to eq. (9) is given. From Fig. 1 it can be concluded that, although these reversible and irreversible reaction are not related, the curves for the enhancement factor vs the *Ha* number for reversible reactions with increasing equilibrium constant show a remarkable similarity with the results for the enhancement factor for irreversible reactions with increasing asymptotic enhancement factors.

The concept of the present paper is that the relation of van Krevelen and Hoftijzer, or similar relations applicable to irreversible reactions, can be extended to reversible reactions and chemically loaded solutions if the asymptotic enhancement factor in these relations is adapted to these conditions. [See also Danckwerts, (1970)]. Because of the explicit description of the enhancement factor, the relation of DeCoursey (1974) for irreversible reactions [eq. (9)] is attractive for this purpose, and will in the present contribution serve as a basis in order to calculate the enhancement factor for reversible reactions in chemically loaded solutions with unequal diffusivities.

The present relation simply states that the reversibility of the reaction, chemical loading and diffusivities of components A, B, C and D primarily affect the value of the asymptotic enhancement factor. Once this influence on the asymptotic enhancement factor is known, the enhancement factor can be calculated with eq. (9) as if the reaction proceeds irreversibly. In Fig. 2 numerical results for the enhancement factor according to the penetration theory are given for very different absorption conditions (i.e. the equilibrium constant K was varied from 0.1 to 10,000), however, the numerical asymptotic enhancement factor was for every equilibrium constant kept constant at 51 by adapting the concentration of B in the bulk. In Fig. 2 it can be seen that the numerically calculated enhancement factors are almost identical over the entire Ha_A range except when the enhancement factor approaches the asymptotic enhancement factor. Also in this figure the enhancement factor according to the relation of DeCoursey (1974) (valid for irreversible reactions) is given for the same asymptotic enhancement factor. Also these enhancement factors only deviate slightly from the numerically calculated ones, the difference being larger in the transition regime from $E_a = Ha_A$ to $E_{a,\infty}$. This agreement seems to confirm the idea that the approximate solution for an irreversible reaction [of e.g. DeCoursey (1974)] can be used as long as the asymptotic enhancement factors needed in these approximations is replaced by the one for the reversible reaction.

Unfortunately, no analytical solution for the asymptotic enhancement factor according to the surface renewal model, for which eq. (9) is valid, is available for reversible reactions and unequal diffusivities

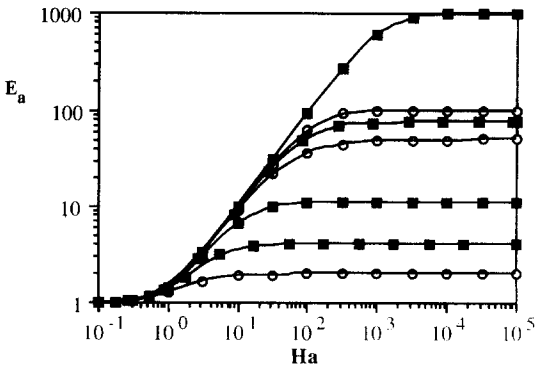

Fig. 1. Similarity for the plot for the reaction A + B ⇔ C + D (reaction orders in all components equal to 1) with varying equilibrium constant (lines with open points; numerical results) and the irreversible reaction A + B ⇒ C + D [results according to eq. (9)] with varying ratio of $[B]_L/(m_a[A]_g)$ (lines with black squares). Lines with open points: $K_{eq} = 0.001$; 0.1 and 1.10^5 from bottom to top respectively; chemical loading = 0.001, $[B]_L = 1000$ mol m^{-3}. Lines with black squares: $[B]_L/(m_a[A]_g) = 3$, 10, 75 and 1000, from bottom to top respectively. All diffusivities for both reactions equal to 1×10^{-9} m^2 s^{-1}, $[A]_i = 10$ mol m^{-3}.

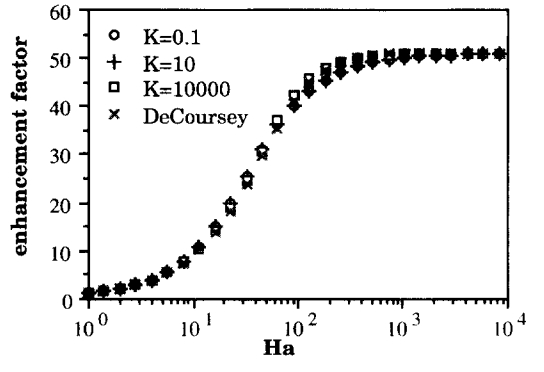

Fig. 2. Influence of the equilibrium constant on the curve of E_a versus Ha_A for the reaction A + B ⇔ C + D for a chemical loading of zero. The numerical asymptotic enhancement factor was kept identical at 51 for all equilibrium constants by changing the concentration of B in the bulk.

in partially converted solutions. However, for these conditions Olander (1960) presented an analytical solution for ($\gamma_a = \gamma_b = \gamma_c = \gamma_d = 1$) for the film model in the instantaneous absorption regime. In 1967, Secor and Beutler obtained an analytical solution for the same conditions in the mass transfer controlled absorption regime for the film model for reaction (1) which allowed for arbitrary stoichiometric coefficients. The relation of Secor and Beutler for reaction (1) is given by

$$E_{a,\infty} = 1 + \frac{\gamma_a D_c}{\gamma_c D_a} \frac{([C]_i - [C]_L)}{(m_a[A]_g - [A]_L)} \quad (10)$$

where $[C]_i$ has to be calculated from relations (11)–(13).

$$[B]_i = [B]_L + \frac{\gamma_b D_c}{\gamma_c D_b} ([C]_L - [C]_i) \quad (11)$$

$$[D]_i = [D]_L + \frac{\gamma_d D_c}{\gamma_c D_d} ([C]_i - [C]_L) \quad (12)$$

$$K = \frac{[C]_i^{\gamma_c} [D]_i^{\gamma_d}}{(m_a[A]_g)^{\gamma_a} [B]_i^{\gamma_b}}. \quad (13)$$

Although eqs (11)–(13) can be solved easily with a root finding procedure, Secor and Beutler also derived an explicit solution for arbitrary γ_a and $\gamma_b = \gamma_c = \gamma_d = 1$ (the solution for $\gamma_a = \gamma_b = \gamma_c = \gamma_d = 1$ was already presented by Olander) and arbitrary γ_a with $\gamma_b = 2$ and $\gamma_c = \gamma_d = 1$. The required equilibrium concentrations in these relations can be derived with an appropriate model able to calculate the equilibrium composition.

3. SIMULATIONS

The simulations were carried out for the following first-order reactions in the absorbing component A:

$$A + B \Leftrightarrow C + D, \quad K = \frac{[C][D]}{[A][B]},$$

$$R_a = -k_{11}[A][B] + k_{-1-1}[C][D] \quad (14)$$

$$A + B \Leftrightarrow C, \quad K = \frac{[C]}{[A][B]},$$

$$R_a = -k_{11}[A][B] + k_{-1}[C] \quad (15)$$

$$A + 2B \Leftrightarrow C + D, \quad K = \frac{[C][D]}{[A][B]^2},$$

$$R_a = -k_{12}[A][B]^2 + k_{-1-1}[C][D]. \quad (16)$$

The results of these calculations are reported in Section 4.2. In Section 4.3 results are also given for reactions (17)–(19) which are second-, third- and zeroth order in A, respectively.

$$2A + B \Leftrightarrow C + D, \quad K = \frac{[C][D]}{[A]^2[B]},$$

$$R_a = -2(k_{21}[A]^2[B] - k_{-1-1}[C][D]) \quad (17)$$

$$3A + B \Leftrightarrow C + D, \quad K = \frac{[C][D]}{[A]^3[B]},$$

$$R_a = -3(k_{31}[A]^3[B] - k_{-1-1}[C][D]) \quad (18)$$

$$A + B \Leftrightarrow C + D, \quad K = \frac{[C][D]}{[A][B]},$$

$$R_a = -k_{01}[B] + k_{-1-1}\frac{[C][D]}{[A]}. \quad (19)$$

It is emphasized that for the reactions (14)–(18) the stoichiometric coefficient of a component was chosen equal to the reaction order in that component. In the backward reaction rate of reaction (19) the product of the concentrations of C and D is divided by the concentration of A in order to fulfil the condition that at equilibrium $R_a = 0$.

For all reactions calculation of the equilibrium composition in the liquid was performed with a simple root finding routine.

The results of the present relation were compared to the results obtained with the exact numerical solution of the model based on the Higbie penetration theory [see, e.g. Versteeg *et al.* (1989)]. Only the numerical simulations which yielded an enhancement factor larger than 1.05 (and only one enhancement factor in the instantaneous absorption regime) were used in the comparisons (see Fig. 3 for a schematic

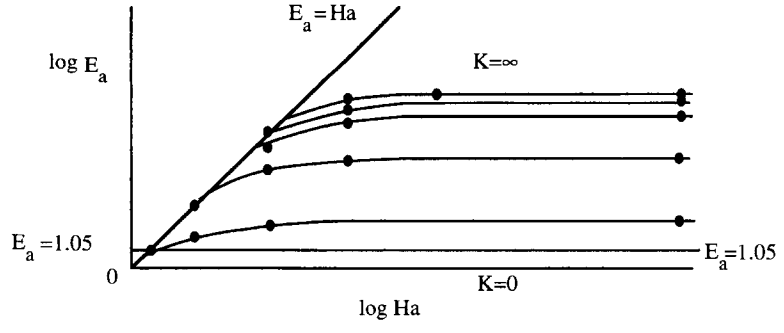

Fig. 3. Schematic presentation of the simulations which were used in the comparison of the numerical model and the two approximations.

Table 1. Process conditions which were used in the comparative simulations

Situation No.	$[B]_{tot}$ (mol m^{-3})	liquid loading	$D_{b,c,d}$ (m^2 s^{-1})	Situation No.	$[B]_{tot}$ (mol m^{-3})	Chem. liquid loading	$D_{b,c,d}$ (m^2 s^{-1})
1	1000	0.001	1×10^{-9}	16	50	0.9	5×10^{-10}
2	1000	0.1	1×10^{-9}	17	1000	0.001	2×10^{-9}
3	1000	0.5	1×10^{-9}	18	1000	0.1	2×10^{-9}
4	1000	0.9	1×10^{-9}	19	1000	0.5	2×10^{-9}
5	50	0.001	1×10^{-9}	20	1000	0.9	2×10^{-9}
6	50	0.1	1×10^{-9}	21	50	0.001	5×10^{-9}
7	50	0.5	1×10^{-9}	22	50	0.1	5×10^{-9}
8	50	0.9	1×10^{-9}	23	50	0.5	5×10^{-9}
9	1000	0.001	5×10^{-10}	24	50	0.9	5×10^{-9}
10	1000	0.1	5×10^{-10}	25	1000	0.5	5×10^{-9}
11	1000	0.5	5×10^{-10}	26	1000	0.5	2×10^{-10}
12	1000	0.9	5×10^{-10}	27	1000	0.001	2×10^{-10}
13	50	0.001	5×10^{-10}	28	1000	0.001	5×10^{-9}
14	50	0.1	5×10^{-10}	29	50	0.001	2×10^{-10}
15	50	0.5	5×10^{-10}	30	50	0.5	2×10^{-10}

Note: In all the simulations $[A]_i = 10$ mol m^{-3}, $D_a = 1\times10^{-9}$ m^2 s^{-1} and $k_L = 1\times10^{-5}$ m s^{-1}.
Enhancement factor was calculated for all situations 1–30 with $K = 1\times10^{-3}$, 0.1, 10, 1×10^{3}, 1×10^{5} and for all these cases with $k_{nm} = 1\times10^{-6}$, 1×10^{-5}, 1×10^{-4}, 1×10^{-3}, 1×10^{-2}, 1×10^{-1}, 1, 10, 1×10^{2}, 1×10^{3}, 1×10^{4}, 1×10^{5} and 1×10^{6} m^3 mol^{-1} s^{-1}. Reaction rate interval for reactions (16) and (18) are from 1×10^{-9}–1×10^{3} and 1×10^{-8}–1×10^{4} respectively.
$[B]_{tot}$ = concentration of B in chemically unloaded solution = [B] + [C] in chemically loaded solution.
Chemical liquid loading defined as total number of moles A and C divided by total number of moles of B and C.
Ha_A number calculated according to eq. (6).

indication). The conditions for the simulations are summarized in Table 1.

4. RESULTS

4.1. *Adaptation of the asymptotic enhancement factor of Secor and Beutler*

In the relations of Secor and Beutler [eqs (10)–(13)] for the asymptotic enhancement factor according to the film model, several diffusivity ratios can be seen. For unequal diffusivities Glasscock and Rochelle (1989) showed that large differences for the asymptotic enhancement factor occur between the film model and surface renewal or penetration theory, respectively. Chang and Rochelle (1982) showed that by using the square root of the diffusivity ratio in the film model, the film- and surface-renewal model give almost the same enhancement factors in the instantaneous absorption regime for the reaction

$$A + B \Rightarrow C.$$

Frank (1996) also adapted the diffusivity ratio in the analytical solution for the film model in the instantaneous absorption region with the square root of these ratios, and verified the results of this (adapted) solution with the exact analytical results obtained for the penetration model for the instantaneous reaction (1). Generally, the modification yielded reasonably good results, however, for some process conditions with unequal diffusivities the deviation could still increase to about 20%. The fact that for these instantaneous irreversible reactions the deviations between the adapted analytical solution of the film model [eq. (20)].

$$E_{a,\alpha} = 1 + \sqrt{\frac{D_b}{D_a}}\frac{[B]_L}{[A]_i} \tag{20}$$

and the exact results according to the penetration theory can increase up to 20% indicates that the often applied expression for the asymptotic enhancement factor for an instantaneous irreversible reaction according to the penetration theory should always be used with care because it is an approximation and not an exact solution.

Blauwhoff (1982) also adapted the diffusivity ratio in the solution of Olander for the film model (valid for instantaneous reversible reactions) with the square root of these ratios, and verified the results of this (adapted) solution for a reaction with a stoichiometric scheme of $\gamma_a = \gamma_b = \gamma_c = \gamma_d = 1$ with the numerical results obtained for the penetration model for reaction (1). Generally, the modification of the solution of Olander yielded reasonably good results, however, as also observed by Frank (1996) for irreversible reactions, the deviations could increase up to 20%.

In this work, the asymptotic enhancement factor according to Secor and Beutler was also adapted in the same way as Blauwhoff did with the solution of Olander, in order to make it more compatible with the penetration and surface renewal theory. For reactions (14) and (18) the results for the asymptotic enhancement factors obtained with the adapted

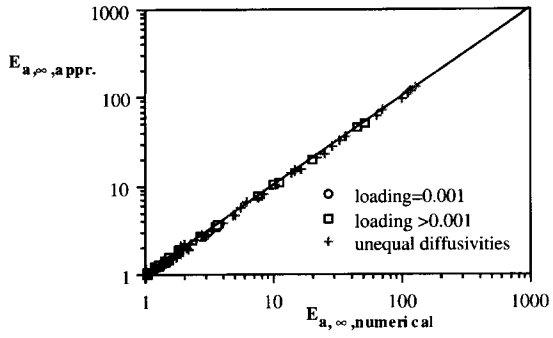

Fig. 4. Asymptotic enhancement factor according to the numerical results of the penetration theory and the adapted solution of Secor and Beutler for reaction (14).

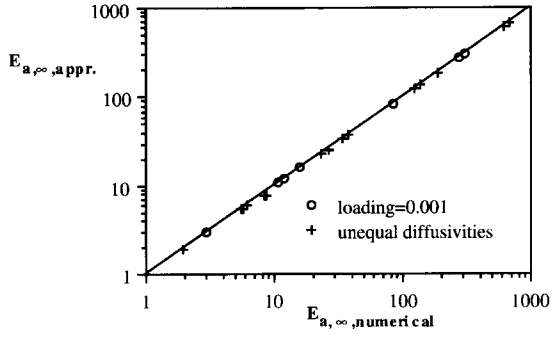

Fig. 5. Asymptotic enhancement factor according to the numerical results according to the penetration theory and the adapted solution of Secor and Beutler for reaction (18).

solution of Secor and Beutler are presented in Figs 4 and 5, respectively.

As can be seen in Figs 4 and 5 the adapted solution of Secor and Beutler seems to predict the asymptotic enhancement factor according to the penetration model well. In general, however, significant differences (for all reactions and situations studied they remained lower than 20%) occur for some cases where the ratio of the diffusivities deviates substantially from one (e.g. 5 or 0.2), while for equal diffusivities the agreement is always within 0.1%.

The value for the approximate enhancement factor according to the present model is calculated by the explicit eq. (9), where the asymptotic enhancement factor in eq. (9) is estimated according eqs (10)–(13), in which the diffusivity ratios are replaced by the square root of these ratios.

Because the present approximation is a combination of the adapted solution of Secor and Beutler and DeCoursey, the present method will further be addressed to as the SBDC model.

4.2. *Results for the SBDC model for first-order reactions in A*

4.2.1. $\gamma_a = \gamma_b = \gamma_c = \gamma_d = 1$. The results of the present SBDC model for reaction (14) are reasonably good (see Table 2). In general, the largest deviations for the SBDC model either occur due to an inaccurate prediction of the asymptotic enhancement factor [for the SBDC model predicted by eqs (10)–(13)] for situations with unequal diffusivities, or, in most situations, as a consequence of a too rapid increase of the enhancement factor in the area $Ha_A > E_a < E_{a,\infty}$. If the maximum deviations are due to an inaccurate prediction of the asymptotic enhancement factor, the replacement of the asymptotic enhancement factor in the SBDC model by the exact numerical result decreases the average deviations substantially (See Table 2). In the area $Ha_A > E_a < E_{a,\infty}$, the SBDC model remains on the line of approximately $E_a = Ha_A$ too long in comparison with the numerical results. It is not surprising that deviations occur for these conditions. Already in Fig. 2 it was observed that for $Ha_A > E_a < E_{a,\infty}$ differences between the numerical results at identical asymptotic enhancement factor and the approximation according to the relation of DeCoursey [eq. (9)] occurred. Substantial maximum deviations (situations 3, 4, 11, 12, 19, 20, 25) are observed for chemical loadings of either 0.5 or 0.9 in combination with $K = 10$. For each of these situations the bulk concentration of A is higher than the interface concentration which means that desorption occurs. One should note that these larger deviations are not due to the fact that desorption takes place, because the deviations observed for equilibrium constants lower than 10 (for which the driving force for desorption is even higher) show a lower deviation.

4.2.2. *Results for* $\gamma_a = \gamma_b = \gamma_c = 1$ *and* $\gamma_d = 0$. For reaction (15) the average deviations for the SBDC model for reactions with equal diffusivities are almost identical as for reaction (14) (Table 3). However, for unequal diffusivities the average deviation increases somewhat. For both situations the maximum deviation is usually negative and mostly occurs for $K = 0.1$. Like for reaction (14), also for this reaction this maximum deviation frequently can be observed as a consequence of a too steep increase of the enhancement factor in the area $Ha_A > E_a < E_{a,\infty}$. Only if the diffusivity ratios are unequal, the maximum deviation also occurs at very high reaction rate constants which indicates that the asymptotic enhancement factor is predicted inaccurately. However, as already mentioned in Section 4.1 this maximum deviation for $E_{a,\infty}$ was always less than 20%. If the approximation for the enhancement factor in the SBDC model is replaced by the numerical value then the average deviation decreases [especially for situation (29) and (30)] substantially as also observed for reaction (14).

4.2.3. *Results for* $\gamma_a = \gamma_c = \gamma_d = 1$ *and* $\gamma_b = 2$. For reaction (16) the Ha_A number was adapted to the kinetic order in component B according to eq. (6) which results in

$$Ha_A = \sqrt{\frac{k_{1,2}[B]_L^2 D_a}{k_L^2}}. \tag{21}$$

Table 2. Results for reaction (14) A + B ⇔ C + D

Situation		SBDC model					
		Deviation					
	n	|average|	max.	K (−)	k_{11} ($m^3\ mol^{-1}\ s^{-1}$)	Deviation for $E_{a,r,SBDC} > 5\%$ for K equal to	Average deviation if $E_{a,r,SBDC} = E_{a,r,numerical}$
1	27	1.650	6.71	0.1	0.001		
2	31	2.048	−9.55	0.1	0.001		
3	30	2.987	−20.5	10	0.01		
4	27	4.243	−27.9	10	0.01		
5	20	1.835	−4.95	10	1		
6	26	1.122	4.53	1×10^5	0.1		
7	24	1.089	4.35	1×10^4	0.1		
8	19	0.854	−4.85	10	0.1		
9	26	2.442	9.28	0.1	0.001		
10	34	1.438	−5.93	10	0.1		
11	27	2.583	−16.8	10	0.01		
12	26	4.112	−21.2	10	0.01		
13	18	3.591	8.55	1000	0.01	$1 \times 10^3, 1 \times 10^5$	1.842
14	22	4.047	8.74	1×10^5	0.1	$1 \times 10^3, 1 \times 10^5$	1.297
15	21	3.984	9.11	1×10^5	0.1	$1 \times 10^3, 1 \times 10^5$	1.051
16	17	2.788	5.64	1×10^5	0.1	$1 \times 10^3, 1 \times 10^5$	0.501
17	23	1.883	5.22	0.1	0.001	-	
18	39	2.369	−13.4	0.1	0.001	-	
19	38	3.028	−24.8	10	0.1	-	
20	27	5.211	−31.5	10	0.001	-	
21	20	1.556	7.70	1000	0.1		
22	30	2.485	5.96	0.1	1×10^6	0.1	1.750
23	33	3.891	7.96	0.1	1×10^6	$0.1, 1 \times 10^3, 1 \times 10^5$	2.229
24	23	5.475	−13.4	1.105	1×10^6	$0.1, 10, 1 \times 10^3, 1 \times 10^5$	3.155
25	37	5.086	−28.2	10	0.1	0.1	5.744
26	26	3.128	6.91	1×10^5	0.1	-	

Note: Conditions for each situation given in Table 1. n = number of simulations which could be used for the specific situation (see Fig. 3). Deviation defined as

$$\text{deviation} = \frac{(E_{a,\text{numerical}} - E_{a,\text{appropriate}})}{E_{a,\text{numerical}}} \times 100\%.$$

With this definition of the Ha_A number the SBDC model gives for equal diffusivities acceptable deviations from the numerically calculated enhancement factors (see Table 4), the deviations being larger in solutions with a chemical loading >0.001 than in solutions with a chemical loading of 0.001. In general, for unequal diffusivities and solutions with a chemical loading of 0.001 the deviations increased [exceptions are situation (23) and (26)]. The maximum deviations mostly do not occur at high reaction rate constants which indicates that the asymptotic enhancement factor is predicted reasonably accurately. Also for this reaction, the maximum deviations in the SBDC model are observed in the area $Ha_A > E_a < E_{a,\infty}$ and occurs, for this reaction and for the situations studied, frequently for almost irreversible reactions. The high average deviation for situation (29) is due to an inaccurate prediction of the asymptotic enhancement factor over the whole range of equilibrium values. If for this situation the asymptotic enhancement factor according to the SBDC model is replaced by the value numerically calculated, the average deviation decreases drastically. Also for some other situations in which the deviation in the approximate asymptotic enhancement factor is higher than 5% this substitution of the approximate asymptotic enhancement factor by the numerical one leads to a decrease in the average deviation [situation (21), (23), (27)].

4.2.4. *Average deviations for reactions first order in the absorbing component* A. In Table 5 a summary of the results for reactions first order in A is given. As it can be seen the results are reasonably good. The lowest deviation is obtained for reaction (14) with a chemical loading of zero. In general the average deviation in Table 5 increases both in the right direction and downwards; i.e. if the absorption conditions start to deviate more and more from the situation the relation of DeCoursey (and therewith the SBDC model) is really meant for, the deviation of the SBDC model starts to increase. It must be noted that for unequal diffusivities the increase in the average deviation is largely due to an inaccurate estimation of the asymptotic enhancement factor according to the

Table 3. Results for reaction (15) A + B ⇔ C

Situation		SBDC model					
		Deviation					
	n	|average|	max.	K ($m^3\ mol^{-1}$)	k_{11} ($m^3\ mol^{-1}\ s^{-1}$)	Deviation for $E_{a,\infty,SBDC} > 5\%$ for K equal to	Average deviation if $E_{a,\infty,SBDC} = E_{a,\infty,numerical}$
1	40	1.904	− 12.4	0.1	1	—	
2	43	1.659	− 6.16	0.1	1	—	
3	39	2.645	− 16.9	0.1	1	—	
4	35	3.856	− 32.7	0.1	1	—	
5	27	1.494	− 5.16	0.1	0.1	—	
6	24	1.592	− 5.11	0.1	0.1	—	
7	25	1.451	− 6.44	0.1	0.1	—	
8	19	1.196	− 7.08	0.1	0.1	—	
21	32	2.604	− 9.27	0.1	0.1	—	
23	33	3.791	− 7.42	1×10^5	1×10^6	$0.1,10,1 \times 10^3,1 \times 10^5$	2.129
25	45	3.774	− 22.9	0.1	1	0.001	3.656
26	37	3.789	− 9.87	0.1	0.1	0.001	1.969
27	38	2.959	7.38	0.001	1×10^6	0.001	1.535
28	47	4.409	− 21.7	0.1	10	0.001	4.226
29	24	11.60	16.8	1×10^5	1×10^6	$0.1,10,1 \times 10^3,1 \times 10^5$	1.734
30	23	11.28	18.2	1×10^5	1×10^6	$0.1,10,1 \times 10^3,1 \times 10^5$	1.315

Note: Conditions for each situation given in Table 1. n = number of simulations which could be used for the specific situation (see Fig. 3).

Table 4. Results for reaction (16) A + 2B ⇔ C + D

Situation		SBDC model					
		Deviation					
	n	|average|	max.	K ($m^3\ mol^{-1}$)	k_{12} ($m^6\ mol^{-2}\ s^{-1}$)	Deviation for $E_{a,\infty,SBDC} > 5\%$ for K equal to	Average deviation if $E_{a,\infty,SBDC} = E_{a,\infty,numerical}$
1	45	4.584	− 18.9	1×10^5	0.001	—	
2	41	5.158	− 18.6	1×10^5	0.001	—	
3	30	3.249	− 17.5	0.1	1×10^{-4}	—	
4	14	4.125	− 11.4	0.1	1×10^{-4}	—	
5	32	2.510	− 10.6	1×10^5	0.001	—	
21	34	7.494	− 21.3	1×10^5	0.01	$10,1 \times 10^3,1 \times 10^5$	4.578
23	20	2.969	7.08	0.1	1×10^3	1×10^{-3},0.1	2.687
26	23	2.230	4.98	1.10^3	1×10^3	—	
27	39	4.669	− 12.3	0.001	1×10^{-6}	0.001	3.707
28	46	6.029	− 21.8	1×10^5	0.001	—	
29	28	9.831	18.3	1×10^5	1×10^3	1×10^{-3},0.1,10, $1 \times 10^3,1 \times 10^5$	1.550

Note: Conditions for each situation given in Table 1. n = number of simulations which could be used for the specific situation (see Fig. 3). Reaction rate varied from 1×10^{-9} to 1×10^3 $m^6.mol^{-2}\ s^{-1}$.

adapted solution of Secor and Beutler. If the asymptotic enhancement factor needed in the SBDC model is taken at the value numerically calculated, the average deviation will decrease for the conditions with unequal diffusivities.

4.3. *Reactions with kinetic order in* A ≠ 1

4.3.1. *Results for* $\gamma_a = 2, 3$ or 0 with $\gamma_b = \gamma_c = \gamma_d = 1$. It is well known that for reactions (17)–(19) the enhancement factor and the Ha_A number are correlated to each other in the interval $2 < E_a \ll E_{a,\infty}$. For the film model this correlation is given by eq. (22) and for the surface renewal model by eq. (23).

Film model:

$$E_a = \frac{Ha_A}{\tanh Ha_A} \approx Ha_A \qquad (22)$$

Table 5. Average deviation for the reactions (14)–(16) according to the SBDC model

Chemical loading diffusivities	0.001 equal	>0.001 equal	0.001 unequal	>0.001 unequal	Overall average deviation
Reaction (14)	1.73 (47)	2.16 (157)	2.33 (87)	3.48 (401)	2.92
Reaction (15)	1.74 (67)	2.20 (185)	4.83 (141)	5.03 (138)	3.58
Reaction (16)	3.72 (77)	4.31 (75)	6.73 (147)	2.57 (43)	5.00

Note: Numbers in brackets indicate the number of simulations.

Surface renewal model:

$$E_a = \sqrt{1 + Ha_A^2} \approx Ha_A. \tag{23}$$

However, for reactions (17)–(19) with $n = 2$, 3 and 0, respectively, neither eq. (22) nor eq. (23) was valid in the regime $2 < E_a \ll E_{a,\infty}$: the enhancement factors calculated with the SBDC model, in which the Ha_A number was defined according to eq. (6), were too low in comparison with the numerical results. Therefore, the Ha_A^2 number was corrected via an adaptive factor, f resulting in the parameter ϕ_A^2 [see eq. (24)], in such a way that eq. (22) was fulfilled in the regime $2 < E_a \ll E_{a,\infty}$.

$$\phi_a = \sqrt{f}\, Ha_A = \sqrt{f}\sqrt{\frac{\gamma_a k_{\gamma_a,1} [A]_i^{n-1} [B]_L D_a}{k_L^2}},$$

$$f = \text{adaptive factor.} \tag{24}$$

For reaction (17) the value of this factor f was 0.675, for reaction (18), 0.503 and for reaction (19), 1.90. (See Fig. 6 and Table 6). Although the resulting ϕ_A number was only derived for the regime $2 < E_a \ll E_{a,\infty}$ it was also used in eq. (9) over the whole Ha_A range in order to approximate the enhancement factor according to the SBDC model.

With these values for the adaptation of the Ha_A number (resulting in the ϕ_A number) a good agreement for the SBDC model and the numerical model was obtained for reactions (17)–(19) for solutions with a chemical loading of 0.001 and both equal diffusivities and unequal diffusivities over the whole Ha_A range. (See Table 7.)

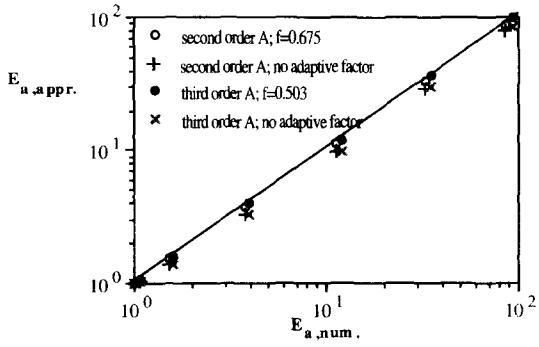

Fig. 6. Parity plot for the numerical enhancement factor for reaction (17) and (18) for situation (1) with $K = 1 \times 10^5$ $[\text{mol m}^{-3}]^{-\gamma_a+1}$ vs the approximate enhancement factor obtained with and without the introduction of the adaptive factor in the Ha_A-number. $E_{a,\infty}$ for reaction (17) = 200.8; $E_{a,\infty}$ for reaction (18) = 300.8.

Also for reactions (17)–(19), the maximum deviations sometimes occurred due to an inaccurate prediction of the asymptotic enhancement factor [see e.g. situation (29)]. If for situation 29 the asymptotic enhancement factor according to the adapted solution of Secor and Beutler in the SBDC model is replaced by the numerically calculated asymptotic enhancement factor the average deviation decreases. Again,

Table 6. Numerical enhancement factor and enhancement factors according to the SBDC model with and without the introduction of the adaptive factor in the Ha_A-number. Conditions as for situation (1) with $K = 1 \times 10^5$ $[\text{mol m}^{-3}]^{-n+1}$ (See also Fig. 6)

Reaction	$E_{a,\infty}$	$E_{a,\text{num}}$	$E_{a,\text{appr.}}$ no adaptation	$E_{a,\text{appr.}}$ with with adaptation
(14)	100.8	3.253	3.281	—
		9.623	9.607	—
(17)	200.8	3.750	3.298	3.781
		11.33	9.873	11.35
		33.86	29.30	33.61
(18)	300.7	3.982	3.304	3.992
		12.09	9.896	12.09
		36.72	30.05	36.48
(19)	100.8	4.455	3.281	4.397
		12.75	9.607	12.96

Table 7. Results for reactions with kinetic order in A unequal to 1

Situation	n	SBDC Deviation |average|	SBDC Deviation max	K	k_{21}	Deviation for $E_{a,\infty,\mathrm{SBDC}} > 5\%$ for K equal to	Average deviation if $E_{a,\infty,\mathrm{SBDC}} = E_{a,\infty,\mathrm{numerical}}$
2A + B ⇔ C + D reaction (17)				K ($m^3 mol^{-1}$)	k_{21} ($m^6 mol^{-2} s^{-1}$)		
1	46	1.54	− 5.73	10	1	—	
5	38	1.05	5.02	0.1	0.001	—	
27	40	2.57	9.13	0.1	1×10^{-3}	—	
28	46	1.66	4.81	0.001	1×10^{6}	—	
29	33	6.79	13.2	1×10^{5}	1×10^{6}	1×10^{-3},0.1,10, 1×10^{3},1×10^{5}	1.45
3A + B ⇔ C + D reaction (18)				K ($m^6 mol^{-2}$)	k_{31} ($m^9 mol^{-3} s^{-1}$)		
1	49	1.58	9.64	0.001	1×10^{-5}	—	
5	40	1.27	− 4.02	0.1	0.01	—	
27	47	1.94	12.9	0.001	1×10^{-5}	—	
28	51	1.62	8.09	0.001	1×10^{-5}	—	
29	38	5.62	10.6	1×10^{5}	1×10^{4}	1×10^{-3},10,1×10^{3}, 1×10^{5}	1.42
A + B ⇔ C + D reaction (19)				K (−)	k_{01} (s^{-1})		
1	46	1.37	7.36	10	1	—	
5	40	0.68	3.31	1×10^{-3}	0.01	—	
27	39	3.67	12.3	0.1	0.01	1×10^{-3},1×10^{-1}	1.88
28	36	2.92	17.3	1×10^{3}	1	—	
29	34	5.21	17.3	1×10^{3}	1×10^{6}	0.1,10,1×10^{3},1×10^{5}	1.84

Note: Conditions for each situation given in Table 1. n = number of simulations which could be used for the specific situation (see Fig. 3). For reactions (17) and (19) reaction rate varied from 1×10^{-6} to 1×10^{6} $m^{3n} mol^{-n} s^{-1}$, for reaction (18) from 1×10^{-8} to 1×10^{4} $m^9 mol^{-3} s^{-1}$.

for most situations the largest deviations occur in the area $Ha_A > E_a < E_{a,\infty}$. It should be noted that the area for which the maximum deviations for reactions (17)–(19) are observed is identical as for reactions (14)–(16) described in Section 4.2.

4.3.2. *Average deviations for reactions with* $n \neq 1$. As can be seen in Table 8 the average deviation of the SBDC model with the introduction of the adaptive factor from the numerical results for a chemical loading of 0.001 is small. As also observed for reactions (14)–(16), this deviation increases if the diffusivities are unequal: however, the results are still good. For solutions with a chemical loading of 0.1, 0.5 or 0.9 the SBDC model gave good results for reactions (17)–(19) as long as the actual concentration of A in the bulk was negligible with respect to the interface concentrations, which means that the reactions are in fact irreversible (results not shown in either Table 7 or Table 8). However, if this concentration was of the same order of magnitude (or even higher in case desorption occurs), the SBDC model gave inaccurate predictions with errors occasionally up to 50% (especially in the range $1 < E_a < 3$). Therefore it is recommended not to use the SBDC for situations in which the bulk concentration of A is of the same order of magnitude as the interface concentration and the order in A is not equal to one.

4.3.3. *The adaptive factor, f, in the* Ha_a *number in the regime* $2 < Ha_A \ll E_{A,\infty}$ *for reactions with* $n \neq 1$. To provide an additional theoretical basis for the adaptive factor in the Ha_A number (resulting in the ϕ_A number) in the regime $2 < Ha_A \ll E_{A,\infty}$ for reactions with identical stoichiometric coefficients and kinetic reaction orders it can be written as

$$\phi_A = \sqrt{f}\, Ha_A = \sqrt{f} \sqrt{\frac{\gamma_a k_{\gamma_a,\gamma_b} [A]_i^{\gamma_a - 1} [B]_L^{\gamma_b} D_a}{k_L^2}}. \quad (25)$$

If $n = 1$ the correction factor, f, is equal to 1, and for $n = 2$, 3 and 0 the correction factor is 0.675, 0.503 and 1.90, respectively (See Section 4.3.1). In the regime $2 < Ha_A \ll E_{A,\infty}$ there is no depletion of B in the

Table 8. Average deviation for reactions (17)–(19) according to the SBDC model; (..) = n

Chemical loading solution diffusivities	0.001 equal	>0.001 equal	0.001 unequal	>0.001 unequal	Overall average deviation
Reaction (17)	1.32 (84)	—	3.38 (119)	—	2.53
Reaction (18)	1.44 (89)	—	2.84 (136)	—	2.29
Reaction (19)	1.06 (85)	—	3.90 (109)	—	2.66

reaction zone, which means that the reaction can be considered as a pseudo nth order reaction in only A, and the Ha_A number is sufficient to correlate the enhancement factor and Ha_A uniquely.

Hikita and Asai (1964) also obtained a kind of Ha_A number in the derivation of the flux. Firstly they treated the irreversible reaction $A \Rightarrow C$ with $R_a = k_n[A]^n$ for the film model [which can be compared to the (numerical) results obtained for $n = 1$, 2 and 3 and $m = 1$ in the regime $2 < Ha_A \ll E_{A,\infty}$]. For this situation, the following relation can be solved analytically:

$$D_a \frac{d^2[A]}{dx^2} = k_n[A]^n, \quad x = 0, \quad [A] = [A]_i,$$

$$x = \delta, \quad [A] = 0. \quad (26)$$

However, they did not introduce a type of dimensionless Ha_A number [defined according eq. (6)] in the dimensionless differential equation [eq. (3)] but in the resulting expression for the concentration gradient of A within the film. The flux at the interface obtained by them is given by:

$$J_a = -D_a \left.\frac{d[A]}{dx}\right|_{x=0} = k_L[A]_i \sqrt{\phi_A^2 + C} \quad (27)$$

with

$$\phi_A^2 = \frac{\frac{2}{n+1} k_n D_a [A]_i^{n-1}}{k_L^2}. \quad (28)$$

ϕ_A is correlated to the Ha_A number [according to eq. (6)] via:

$$\phi_A = \sqrt{\frac{2}{n+1}}\, Ha_A. \quad (29)$$

The constant C in the flux equation is an integration constant which is dependent on ϕ_A and varies between 0 (for high ϕ_A values) and 1 (for low ϕ values). For $n = 0$ or $n = 1$ an analytical expression can be obtained for C, however, for other values of n the value of C has to be calculated numerically.

As already mentioned for high ϕ_A-values and arbitrary n values C becomes zero and disappears, which means that $E_a = \phi_A$. In Section 4.3.1 it was shown that the enhancement factor is correlated to Ha_A in the regime $2 < Ha_A \ll E_{A,\infty}$ by

$$E_a = \sqrt{f}\, Ha_A. \quad (30)$$

This means that for the regime $2 < Ha_A \ll E_{A,\infty}$:

$$f = 2/(n+1). \quad (31)$$

The factor $2/(n+1)$ is equal to 2 for $n = 0$, 1 for $n = 1$, 0.666 for $n = 2$ and equal to 0.500 for $n = 3$. These values are close to the values found for the adaptive factor f in the regime characterized by $2 < Ha_A \ll E_{A,\infty}$ for $n = 0$ ($m = 1$), $n = 1$ ($m = 1$), $n = 2$ ($m = 1$) and $n = 3$ ($m = 1$) which were 1.90, 1, 0.675 and 0.503, respectively (see Section 4.3.1). It should be noted that although the adaptive factor f was taken as a constant over the whole Ha_A range in the SBDC model, it is was only fitted for $2 < Ha_A \ll E_{A,\infty}$ and is strictly only valid in that regime.

4.4. *General remarks*

In general, the SBDC gives reasonably good results for various reactions in comparison to numerical results obtained for the model based on the Higbie penetration theory. Although the average deviation for the SBDC model is always reasonable, the main shortcoming of the SBDC model is that, sometimes, medium deviations can occur. Occasionally, for unequal diffusivities and very high reaction rate constants, the modified relation of Secor and Beutler used to calculate the asymptotic enhancement factor, introduces these deviations, but these discrepancies were smaller than 20% for all reactions and situations studied. The somewhat larger deviations sometimes observed (the maximum deviation found in all 2187 simulations was 30.5%), occur in the range of $Ha_A > E_a < E_{a,\infty}$. In this area as well as for most situations studied, the SBDC model sometimes approaches the asymptotic enhancement factor too rapidly with increasing Ha_A-number in comparison with the numerical results. However, it must be emphasized that the number of simulations which show such a large deviation is small: from a total of 2187 pre-selected simulations (See Fig. 3) only 26 ($\approx$1.18%) had a deviation which was larger than 20%.

Although the approximation was tested for many process conditions, there may, of course, be reaction conditions for which the average deviation is considerably higher (e.g. with unequal diffusivities of all components). Therefore, it should be kept in mind that a deviation is generally caused by:

- an incorrect prediction of the asymptotic enhancement factor according the method of Secor and Beutler caused by unequal diffusivities;

- the transition area $Ha_A > E_a < E_{a,\infty}$;
- equilibrium constants of $K \approx 0.1$–10;
- diffusivity ratios which increasingly differ from 1,
- increasing chemical liquid loadings (especially for $n \neq 1$ where the approximation should not be used).

Therefore, if one wishes to know the exact enhancement factor for a particular model, extensive numerical procedures still have to be performed. However, for most practical cases the SBDC method offers a margin of error which seems acceptable.

5. CONCLUSIONS

A new explicit relation has been proposed for the prediction of the enhancement factor for reversible reactions of finite rate in chemically loaded solutions which also allows for unequal diffusivities. In this contribution a simple explicit relation for the enhancement factor is presented, which is not based on the approximation of the absorption process, but is derived from a similarity which can be observed between the results of the approximation of van Krevelen and Hoftijzer or DeCoursey (1974), and the exact numerical results.

The present relation combines two already existing models of DeCoursey (1974), for irreversible finite rate reactions according to the surface renewal model, and the solution of Secor and Beutler (1967) for the film model for instantaneous reversible reactions. The diffusivity ratios in the equation of Secor and Beutler (1967) were replaced by the square root of these ratios in order to adapt the enhancement factors to the penetration theory.

The results of this new relation was, for various reactions, compared to the numerical enhancement factors obtained for the model based on the Higbie penetration theory. The agreement was reasonably good. The largest average deviations were obtained for solutions with diffusivity ratios not equal to one (which resulted in an incorrect prediction of the asymptotic enhancement factor needed in the SBDC model) and substantial chemical loadings. Replacement of the approximate asymptotic enhancement factor [according to the adapted solution of Secor and Beutler (1967)] in the SBDC model by the numerically calculated asymptotic enhancement factor caused a decrease in the average deviation.

For reactions with a kinetic order of $n = 0$, $n = 2$ or $n = 3$ the Ha_A^2 number had to be multiplied by a factor, f, of 1.90, 0.675 and 0.503, respectively in order to relate the Ha_A number and the enhancement factor in the regime $2 < E_a \ll E_{a,\infty}$ to each other according to the relation $E_a = \sqrt{f}\, Ha_A$. These factors f agreed well with the values theoretically derived by Hikita and Asai (1964) in their dimensionless number. However, it is argued that the dimensionless number of Hikita and Asai (1964) cannot be used to present the results of absorption rate calculations in a unique way.

On account of its explicit nature, the present approximation seems useful for rapid and reasonable prediction of the enhancement factor.

NOTATIONS

[A],[B], [C],[D]	concentration of reactants and products mol m^{-3}
$[A]_i$	concentration of A at the interface mol m^{-3}
$[B]_{tot}$	initial concentration of B in chemically unloaded solution mol m^{-3}
$[B]_L$	actual concentration of B in chemically loaded solution mol m^{-3}
D	diffusion coefficient $m^2\ s^{-1}$
E_a	Enhancement factor dimensionless
$E_{a\infty}$	asymptotic enhancement factor dimensionless
f	adaptive factor in the ϕ_A number dimensionless
Ha_A	Ha_A number [see eq. (7)] dimensionless
J_a	flux of component A mol $m^{-2}\ s^{-1}$
K	equilibrium constant $[\text{mol m}^{-3}]^{-\gamma_a-\gamma_b+\gamma_c+\gamma_d}$
k_L	liquid side mass transfer coefficient $m\ s^{-1}$
k_{nm}	forward reaction rate coefficient $[m^{-3}\ mol^1]^{1-n-m}\ s^{-1}$
m_a	partition coefficient of gas A dimensionless
n	number of simulations dimensionless
γ_i	in this paper: Stoichiometric coefficient, and also kinetic order of component i dimensionless
ϕ_A	reaction number number defined by eq. (32) dimensionless

Subscripts

i	interfacial
L	in the liquid

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